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A Revision of the Linear-Dashpot Model Applied in PFC

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Abstract

This paper investigates the contact model applied in the Distinct Element Method (DEM). The linear – dashpot model implemented in the commercial software PFC3d (Particle Flow Code in three dimensions, version 3.0) is investigated. The contact model is solved numerically by applying Newton's second law of motion and a force – displacement law, which describes the particle – particle and particle – wall collisions. The numerical results obtained with PFC are compared with the analytical solution and numerical solution with Matlab. Our numerical results show that the contact model in PFC is not properly implemented, i.e. the effective mass is calculated as the arithmetic mean of the masses of two colliding particles.

Keywords: Coefficient of restitution, DEM, Effective mass,
Linear dashpot model, Particle collisions, PFC

1. Introduction

The definition of the contact model is crucial for the Distinct Element Method. Figure 1 presents the collision detection between two particles, identifiable by a positive particle overlap $\xi > 0$. If the collisions are assumed to be linear, the contact model is usually defined by a Kelvin – Voigt model. This model is represented by a purely viscous damper and a purely elastic spring connected in parallel. Figure 2 shows the linear dashpot model applied to the collision of two particles. The contact model is active, if two particles are physically in contact.

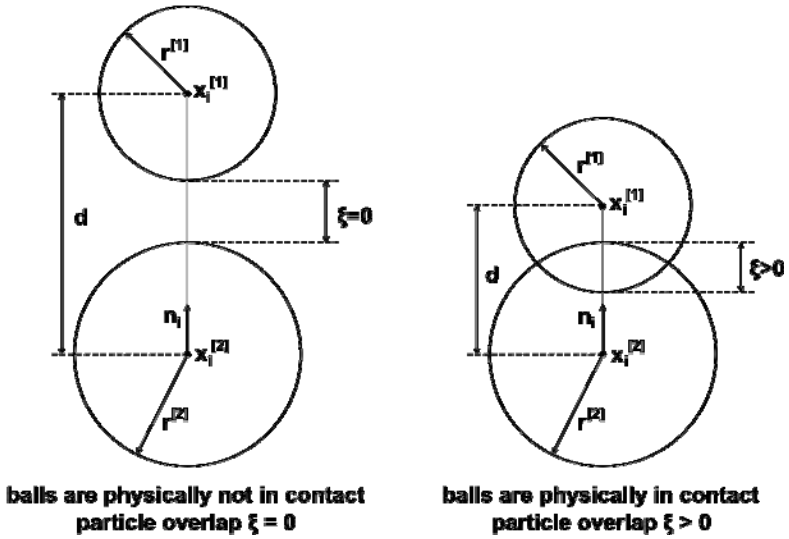

Figure 1: Presentation of a particle – particle contact

Since the presented paper is focused on the calculation of the effective mass, it suffices to study collisions in normal direction. The particle rotation and shear force is not considered.

2. Analytical solution of linear – dashpot model

In order to obtain the analytical solution of the linear dashpot model the system of two freely moving particles is mapped to a Kelvin – Voigt model. The system of two colliding balls is simplified to a one particle system, where one end of the Kelvin – Voigt model is fixed and the other one is free in translation. Figure 2 presents the relation between the two – particle model and the equivalent one particle model. Furthermore the relation between the ball – stiffness and the spring stiffness used at the Kelvin – Voigt model are given in Figure 2. If the two particles have the stiffness $k^{[1]}$, $k^{[2]}$ the related spring stiffness k of the Kelvin – Voigt model can be shown to be:

$$k = \frac{k^{[1]} \cdot k^{[2]}}{k^{[1]} + k^{[2]}}$$

The viscous damper c is parallel to the spring k.

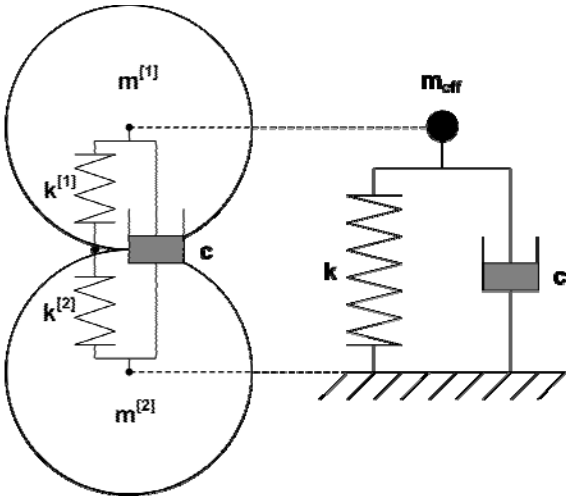

Figure 2: Equivalent one particle system related to the two particle linear dashpot model

The governing differential equation of the one particle system can be written out as follows:

$$m_{eff}\,\ddot{\xi} + c\,\dot{\xi} + k\,\xi = 0 \tag{1}$$

where $\xi(t)$ is the particle overlap, which is equal to the compression of the Kelvin-Voigt model. The initial conditions are defined as

$$\xi(0) = 0 \quad \text{and} \quad \dot{\xi}(0) = v_0 \tag{2}$$

Where v_0 is the relative velocity of the two particles at the beginning of the collision $(t = 0)$, measured in normal direction $\vec{n}$. The particle overlap can be further related to the particle geometries through:

$$\begin{aligned} \xi(t) &= \max(0, r^{[1]} + r^{[2]} - d) \\ d &= \left| x_i^{[1]} - x_i^{[2]} \right| \end{aligned} \tag{3}$$

The effective mass m_{eff} of the system is defined as the half of the geometric mean of the two particles ([2],[17],[18],[5]):

$$m_{eff} = \frac{m^{[1]} m^{[2]}}{m^{[1]} + m^{[2]}} \tag{4}$$

The solution of equation (1) can be solved together with the initial conditions in (2) to give

$$\xi(t) = v_0\, m_{eff} \left(\frac{e^{\left(-c+\sqrt{c^2-4k\,m_{eff}}\right)\frac{t}{2m_{eff}}}}{\sqrt{c^2-4k\,m_{eff}}} - \frac{e^{-\left(c+\sqrt{c^2-4k\,m_{eff}}\right)\frac{t}{2m_{eff}}}}{\sqrt{c^2-4k\,m_{eff}}} \right) \tag{5}$$

By using the following terms, equation (5) can be simplified to equation (7a) and (7b).

$$\omega_0 = \sqrt{\frac{k}{m_{eff}}}; \quad \beta = \frac{c}{2m_{eff}}; \quad \omega = \sqrt{\omega_0^2 - \beta^2};$$
$$\alpha = \beta/\omega_0; \quad \Omega = \sqrt{\beta^2 - \omega_0^2} = i \cdot \omega; \tag{6a}$$

ω_0 is the natural frequency of the spring. c is the damping parameter of the viscous damper and c_c the critical damping parameter. The critical damping can be obtained, when the square roots in the denominator of equation (5) becomes zero, i.e.:

$$\sqrt{{c_c}^2 - 4k\,m_{eff}} = 0$$
$$\Rightarrow \quad c_c = 2\sqrt{k\,m_{eff}} = 2m_{eff}\sqrt{\frac{k}{m_{eff}}} = 2\,m_{eff}\,\omega_0 \tag{6b}$$

α is called the critical damping ratio and is defined as the ratio between damping and critical damping:

$$\alpha = \frac{c}{c_c} = \frac{\beta}{\omega_0} \tag{6c}$$

Another important relation is given between the viscous damping c, the critical damping ratio α, the effective mass m_{eff} and the stiffness k.

$$c = 2\alpha\sqrt{m_{eff}\,k} \tag{6d}$$

If $(\omega_0^2 - \beta^2 > 0) \Leftrightarrow (\alpha < 1)$ the system is low damped and equation (5) can be simplified to:

$$\xi(t) = \frac{v_0}{\omega} e^{-\beta t} \sin(\omega t) \quad if\ \beta < \omega_0 \tag{7a}$$

If $(\omega_0^2 - \beta^2 < 0) \Leftrightarrow (\alpha > 1)$ the system is highly damped and the ω becomes complex. In order to transform equation (7a) into a function with real arguments, ω is replaced by Ω and the function sine by hyperbolic sine to give:

$$\xi(t) = \frac{v_0}{\Omega} e^{-\beta t} \sinh(\Omega t) \quad if \ \beta > \omega_0 \tag{7b}$$

with:

$$-i \cdot \sin(i \cdot x) = \sinh(x)$$

If $\alpha < 1$, the impact duration t_c can be derived by the calculation of the smallest root of equation (7a).

$$\xi(t_c) = 0; \quad t_c > 0 \tag{8}$$

From this it follows that:

$$t_c = \pi / \omega \tag{9}$$

If $\alpha > 1$, equation (7b) has no other root than $t_c = 0$. This means that the two particles remain together forever.

The coefficient of restitution ε is defined as the ratio of impact velocity to rebound velocity. This coefficient is closely related to the critical damping ratio α. If $\varepsilon = 1$ the impact is perfectly elastic, if $\varepsilon = 0$ the impact is totally inelastic. Since the properties of granular materials often provide information about the coefficient of restitution but not about the critical damping ratio, the relation between α and ε are given below

$$\varepsilon = \frac{\dot{\xi}(t_c)}{\dot{\xi}(0)} = e^{-\beta \frac{\pi}{\omega}} = e^{-\frac{\alpha \pi}{\sqrt{1-\alpha^2}}} \tag{10}$$

Equation (10) is only valid if $\alpha < 1$. The inverse function of equation (10) can be easily shown to be:

$$\alpha = -\frac{\ln(\varepsilon)}{\sqrt{\ln^2(\varepsilon) + \pi^2}} \tag{11}$$

The equations (6a)-(6d) show that the impact behavior is strongly dependent on the effective mass in the contact model. It seems that the effective mass given in equation (4) is not used in PFC. Rather, the contact model in PFC is based on the arithmetic mean of the two colliding particles, i.e.

$$m_{eff} = \frac{m^{[1]} + m^{[2]}}{2} \tag{12}$$

For evaluation purposes the impact force $F = m_{eff} \cdot \ddot{\xi}(t)$ and the compression of the Kelvin – Voigt model $\xi(t)$ are compared. In the case of low damping $(\alpha < 1)$ the

force can be calculated by the second derivative of equation (7a) multiplied with the effective mass m_{eff}

$$\begin{aligned} F_{analyt} &= m_{eff} \cdot \ddot{\xi}(t) \\ &= \frac{m_{eff} v_0}{\omega} \left(\beta^2 e^{-\beta t} \sin(\omega t) - \omega^2 e^{-\beta t} \sin(\omega t) - 2\omega\beta e^{-\beta t} \cos(\omega t) \right) \end{aligned} \tag{14a}$$

In the case of high damping $(\alpha > 1)$ the force is calculated by the second derivative of equation (7b)

$$\begin{aligned} F_{analyt} &= m_{eff} \cdot \ddot{\xi}(t) \\ &= \frac{m_{eff} v_0}{\Omega} \left(\beta^2 e^{-\beta t} \sinh(\Omega t) + \Omega^2 e^{-\beta t} \sinh(\Omega t) - 2\Omega\beta e^{-\beta t} \cosh(\Omega t) \right) \end{aligned} \tag{14b}$$

3. Validity of analytical solution

A comparison between the analytical solution and PFC with reference to the impact force and the particle overlap can be made only if the masses of the two balls $i, (i = 1,2)$ are equal to the effective mass, i.e. $m^{[i]} = m_{eff}$. The calculation cycle is divided into two parts:

1.) the calculation of the impact force (law of motion) and
2.) the calculation of particle motion, caused by the impact force (Newton's second law).

The law of motion is implemented in PFC as:

$$F_{PFC} = -c\dot{\xi} - k\xi \tag{15}$$

Newton's second law is given by:

$$F_{PFC} = m^{[i]} \left(\ddot{\xi}^{[i]} - g \right) \Rightarrow \ddot{\xi}^{[i]} = \frac{F_{PFC}}{m^{[i]}} + g \tag{16}$$

In a first step in PFC, the forces are calculated by equation (15). The solution of equation (15) is inserted into equation (16). Newton's second law is transformed in order to obtain the acceleration $\ddot{\xi}^{[i]}$ as a function of the particle mass $m^{[i]}$ and the gravitational acceleration g of particle $i, (i = 1,2)$. After the calculation of the particle acceleration, the displacement can be obtained by a finite difference scheme.

In comparison to PFC, the analytical solution evaluates at first the particle displacements $\xi(t)$ as a closed solution (equations (7a) and (7b)) of the Kelvin – Voigt model (equation (1)). The analytical solution can be compared to the PFC solution if the following conditions from equations (17) and (18) are satisfied.

The left hand side of equation (17) represents the force term of the Kelvin – Voigt model.

$$\underbrace{m_{eff}\,\ddot{\xi}}_{F_{analyt}} = -c\,\dot{\xi} - k\,\xi \tag{17}$$

The comparison of the analytical and the numerical solution (equation (18)) shows that the two forces are only equal if $g = 0$ and $m^{[i]} = m_{eff}$:

$$\underbrace{m^{[i]}\left(\ddot{\xi}^{[i]} + g\right)}_{F_{PFC}} = \underbrace{m_{eff}\,\ddot{\xi}}_{F_{analyt}} \tag{18}$$

Based on the derivation of the range of validity it can be shown that the analytical solution can be compared to the numerical scheme if the following conditions of the ball masses $m^{[i]}, i = 1,2$ are satisfied:

Case 1: If the effective mass is calculated by equation (4), the condition $m^{[i]} = m_{eff}$ is only satisfied if:

$$m_i = \frac{m^{[1]} \cdot m^{[2]}}{m^{[1]} + m^{[2]}} \Leftrightarrow m^{[i]} = 0 \tag{19}$$

Case 1: If the effective mass is calculated by equation (12) the analytical solution can be compared to the numerical scheme if:

$$m_i = \frac{m^{[1]} + m^{[2]}}{2} \Leftrightarrow m^{[1]} = m^{[2]} \tag{20}$$

From equation (19) it follows that the analytical solution is not applicable if the effective mass is calculated by equation (4).

4. Matlab implementation of the numerical scheme

If a comparison between the analytical solution and PFC cannot be made for arbitrary particle masses, the numerical solution with Matlab is used instead of the analytical solution. The Matlab code follows the numerical scheme of PFC but

allows a user defined choice of the effective mass. Besides the handling of arbitrary ball masses, gravitation acceleration can be taken into consideration.

```
%-------------------------------------------------------------------------
dt=0.001;                       % time step
time=0:dt:0.12;

xpos=0.0;                       % ξ(0) = 0
xvel=-2.0;                      % ξ̇(0) = v0
m1=15;                          % mass of ball 1
m2=5;                           % mass of ball 2
kn1=1e4;                        % stiffness of ball 1
kn2=1e4;                        % stiffness of ball 2
alpha=0.5;                      % critical daming ratio
g=0;                            % gravitational acceleration

k=kn1*kn2/(kn1+kn2);            %
m=(m1+m2)/2.0;                  % effective mass
c=2.0*sqrt(k*m)*alpha;          % damping constant

%----- numerical calculation -----
F=0;
n=1;
for t=time(2:end)
   xvel(n+1)=xvel(n)+(F(n)./(m1)+g).*dt;
   xpos(n+1)=xpos(n) + xvel(n+1)*dt;
   if xpos(n+1) < 0
      xi  = xpos(n+1);
      xi_p = xvel(n+1);
      F(n+1)=-k*xi - c*xi_p;
   else
      F(n+1)=0;
   end
   n=n+1;
end
%-------------------------------------------------------------------------
```

5. Comparison between PFC and own results

The following case studies compare the numerical Matlab solution with the numerical PFC solution. If the initial conditions are within the range of validity the numerical solutions can also be compared to the analytical solution.

Case study 1
The first case study represents a low damped system. The masses of both balls are equal and the gravitational acceleration is zero. The following parameters are used in all solutions.

$$v_0 = -2$$
$$m^{[1]} = 5$$
$$m^{[2]} = 5$$
$$k^{[1]} = 10000$$
$$k^{[2]} = 10000$$
$$\alpha = 0.5$$
$$g = 0$$

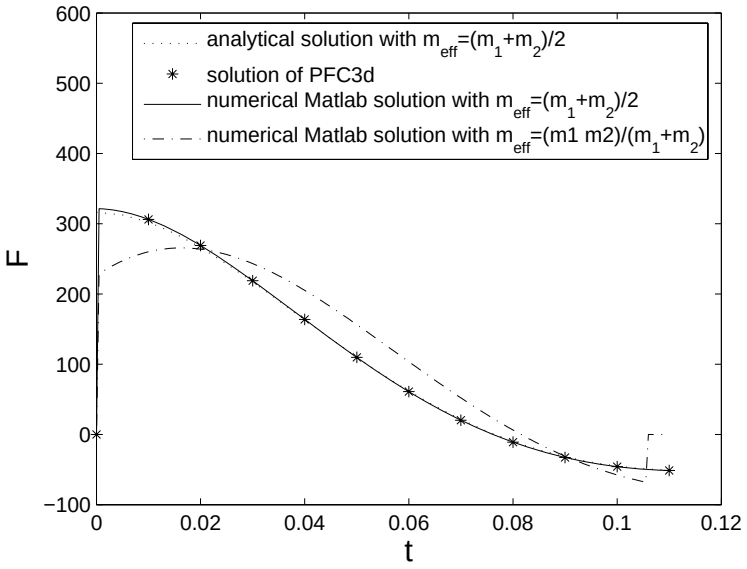

Figure 3: Comparison between analytical solution, Matlab solution and PFC solution of the impact forces $F(t)$, calculated with the two different types of effective masses.

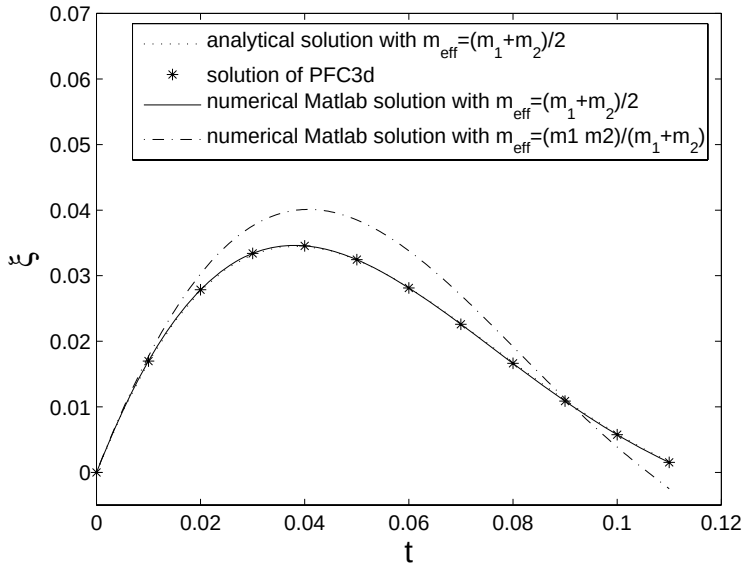

Figure 4: Comparison between analytical solution, Matlab solution and PFC solution of the particle overlap $\xi(t)$, calculated with the two different types of effective masses.

Case study 2

The second case study represents a highly damped system. The masses of both balls are equal and the gravitational acceleration is set to zero. The following parameters are used in all calculations.

$$v_0 = -2$$
$$m^{[1]} = 5$$
$$m^{[2]} = 5$$
$$k^{[1]} = 10000$$
$$k^{[2]} = 10000$$
$$\alpha = 2.0$$
$$g = 0$$

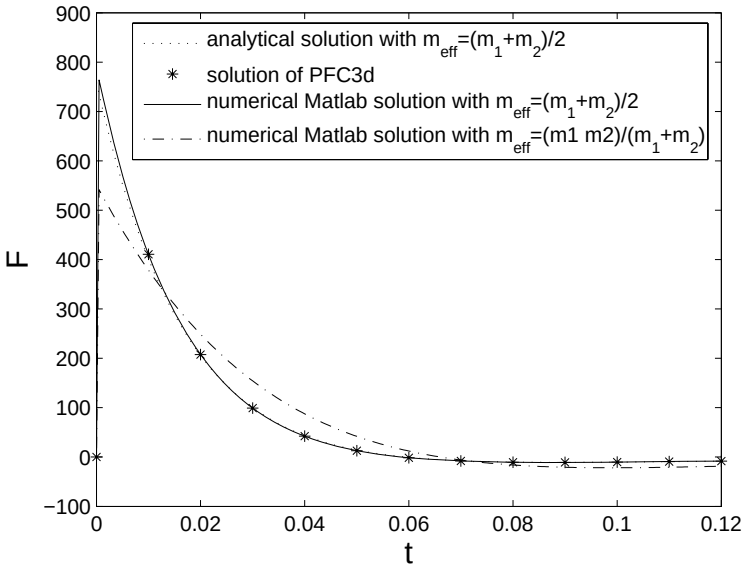

Figure 5: Comparison between analytical solution, Matlab solution and PFC solution of the impact forces $F(t)$, calculated with the two different types of effective masses.

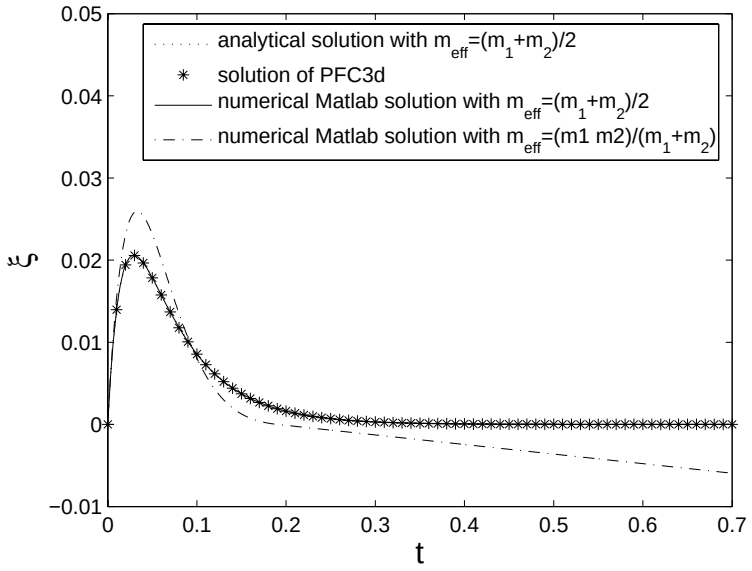

Figure 6: Comparison between analytical solution, Matlab solution and PFC solution of the particle overlap $\xi(t)$, calculated with the two different types of effective masses.

In Figures 3-6 the analytical solutions, numerical Matlab solutions are compared with the results obtained form PFC3d version 3.0. Figure 3 to Figure 6 shows that the Matlab solution based on the effective mass $m_{eff} = m^{[1]} \cdot m^{[2]} / (m^{[1]} + m^{[2]})$ clearly differs from the analytical solution and the Matlab solution based on the effective mass $m_{eff} = (m^{[1]} + m^{[2]}) / 2$. The solution obtained from PFC3d v3.0 fits the analytical and numerical solution based on the effective mass obtained by the arithmetic mean.

Case study 3

The third case study represents a low damped system with different ball masses $m^{[1]} \neq m^{[2]}$ and a gravitational acceleration of $g = 9.81$ m/s^2. The analytical solution is not valid regarding to these conditions. However, the PFC results can be compared to the numerical scheme implemented in Matlab. The following parameters are used for both PFC and Matlab calculations.

$$v_0 = -2$$
$$m^{[1]} = 5$$
$$m^{[2]} = 15$$
$$k^{[1]} = 10^5$$
$$k^{[2]} = 10^6$$
$$\alpha = 0.4$$
$$g = 9.81$$

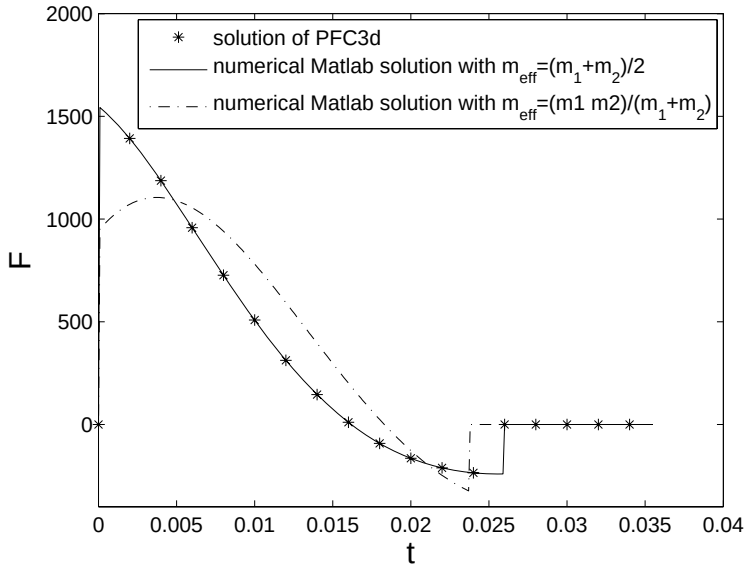

Figure 7: Comparison between Matlab solution and PFC solution of the impact forces $F(t)$, calculated with the two different types of effective masses.

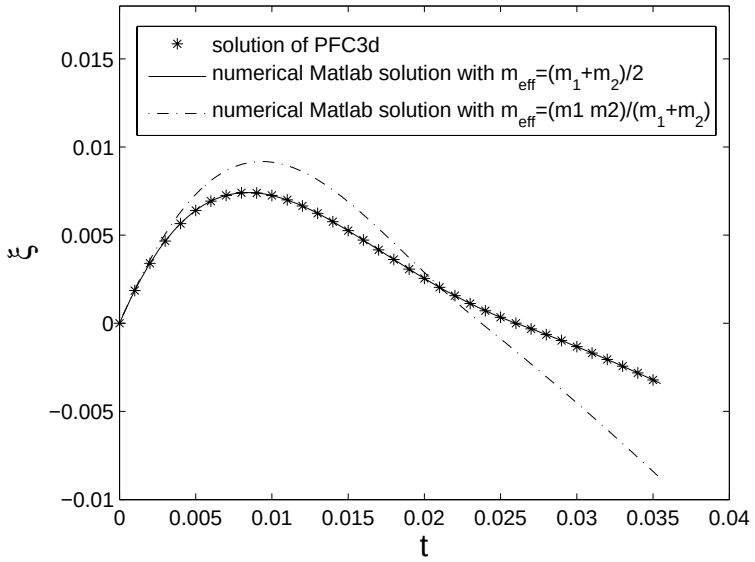

Fig 8: Comparison between Matlab solution and PFC solution of the particle overlap $\xi(t)$, calculated with the two different types of effective masses.

In Figs. 7 and 8 numerical Matlab solutions based on the two different effective mass are compared with the PFC results. In both figures the PFC results fits the numerical Matlab solution based on the effective mass calculated as $m_{eff} = (m^{[1]} + m^{[2]})/2$. On the other hand, the Matlab solution based on $m_{eff} = m^{[1]} \cdot m^{[2]} / (m^{[1]} + m^{[2]})$ significantly differs from the other solutions.

6. Conclusion

Our numerical results confirm the assumption that the effective mass used in PFC3d version 3.0 [6] is calculated by the arithmetic mean of the masses of the two colliding balls, which is at odd with the well known definition of effective mass, namely the geometric mean. This difference in the definition of the effective mass is very important for the calculation of force peaks, collision times and the coefficient of restitution which is often related to the collision behavior of granular matters.
The appropriate choice of the effective mass definition is a crucial part of the Distinct Element Method because the relation between restitution coefficient, particle stiffness, damping constant, critical damping ratio and ball masses is strongly dependent on it. It is to be hoped that this will be corrected in the next version of PFC3d.

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